Computational Advances in Drug Discovery

September 23-26, 2019

Convento dell'Annunziata,
Sestri Levante (GE), Italy

Organizing Committee

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23 September 2019

09:00 - 10:00	Registration and Welcome
Session 1	**Computations and drug design**
10:00 - 10:30	From phosphate catalytic reaction mechanisms to drug unbinding *Edina Rosta, King's College London*
10:30 - 11:00	Adaptive Monte Carlo Techniques for Drug Design *Victor Guallar, BSC, Barcelona*
11:00 - 11:30	Coffee break
11:30 - 12:00	Exploration of Molecular Recognition Processes Using Machine Learning *Kenneth Merz, Michigan State University*
12:00 - 12:30	GPUs, GUIs, TI, AI, Oh My! *Ross Walker, GSK, USA*
12:30 - 13:00	Confronting Challenging Innate Immune Targets Using Integrated Biophysics and Simulation *Woody Sherman, Silicon Therapeutics, USA*
13:00 - 15:00	Lunch
15:00 - 15:30	Exploiting allostery for computer-aided drug design on oncogenes *Zoe Cournia, Academy of Athens*
15:30 - 16:00	The ANI family of deep learned potentials: development, application to general computational chemistry problems, and future prospects *Adrian Roitberg, University of Florida*
16:00 - 16:30	Coffee break
16:30 - 17:00	Theories, Methods, and Software for Free Energy-Based Virtual Screening *Emilio Gallicchio, Brooklyn College, USA*
17:00 - 17:30	New Validation Strategy for Benchmarking Virtual Screening Methods based on High-Throughput Screening (HTS) Data *Steven Jerome, Schrödinger*
17:30 - 19:30	Poster Session and Cocktail Party

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Session 2	Computations and drug design
09:30 - 10:00	Probing the role of hydration in protein-ligand binding via biased MD *Walter Rocchia, Istituto Italiano di Tecnologia*
10:00 - 10:30	Fragment and Mini Fragment screening applied to ERK1/2 Kinase *Valerio Berdini, Astex, Cambridge, UK*
10:30 - 11:00	Coffee break
11:00 - 11:30	Multiscale simulation of drug binding and enzyme inhibition *Adrian Mulholland, University of Bristol*
11:30 - 12:00	FMAP: the Funnel-Metadynamics Automated Protocol for ligand binding free-energy calculations *Vittorio Limongelli, USI – Switzerland*
12:00 - 12:30	Combining Machine Learning and Metadynamics for Absolute Binding Free Energies *Francesco L. Gervasio, UCL, London*
12:30 - 18:00	Free time
Keynotes	
18:00 - 18:45	Machine learning and molecular dynamics *Michele Parrinello, ETH Zurich, IIT*
18:45 - 19:30	Computer-Aided Discovery of Enzyme Inhibitors *William Jorgensen, Yale University*

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Session 3	Computations and drug design
09:30 - 10:00	Multiscale models of the CRISPR-Cas9 genome editing system *Giulia Palermo, UC Riverside*
10:00 - 10:30	Can we tame by simulation the nucleation of Molecular Crystals? *Giovanni Ciccotti, University of Roma "La Sapienza"*
10:30 - 11:00	Coffee break
11:00 - 11:30	Novel ligands targeting RNA in neurodegenerative diseases by molecular simulation *Paolo Carloni, FZJ, Julich, Germany*
11:30 - 12:00	Protonation, Charges, pKa: Nightmare for Computational Drug Design *Gerhard Klebe, Philipps-University of Marburg*
12:00 - 12:30	Enzyme inhibitor design driven by free-energy simulations *Alessio Lodola, University of Parma*
12:30 - 14:30	Lunch
14:30 - 15:00	EDES: an enhanced-sampling MD-based protocol for molecular docking *Attilio Vittorio Vargiu, University of Cagliari*
15:00 - 15:30	Targeting the folding of oncogenic proteins by predicting their local unfolding status *Giorgio Colombo, University of Pavia*
15:30 - 15:50	Dynamics of catalytic residues and metals through the stages of group II intron splicing *Jacopo Manigrasso, IIT (Short Talk)*
15:50 - 16:30	Coffee break
16:30 - 17:00	Computational investigations of TRP channels modulation by phospholipids, toxins and small molecules *Eleonora Gianti, Temple University*
17:00 - 17:30	Metallo-biology of diseases as revealed from multiscale-simulations *Alessandra Magistrato, CNR Trieste, SISSA*

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Session 4	Computations and drug design
09:30 - 10:00	Probing the role of hydration in protein-ligand binding via biased MD *Giulia Rossetti, RWTH Aachen, Germany*
10:00 - 10:20	A third metal ion in human exonuclease 1: recruiting mechanism and functional role investigated via MD simulations *Elisa Donati, IIT (Short Talk)*
10:20 - 11:00	Coffee break
11:00 - 11:30	Structural and functional characterisation of the KRAB-domain associated protein 1 *Giulia Fonti, EPFL, Lausanne*
11:30 - 12:00	Trypanosomicidal ariloxy quinones, trypanothione reductase and glucose 6-fosfate dehydrogenase: multiple and multitargetted action studies *Margot Paulino Zunini, DETEMA, UdelaR*
12:00 - 12:30	From kinetics of protein-ligand [un]binding to absolute binding free energy: towards a unifying computational framework *Sergio Decherchi, IIT*
12:30 - 13:00	Closing Remarks